Theoretical Study of Electron Scattering from Magnesium Sulfide

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Introduction

- Magnesium sulfide (MgS) is the first metallic sulfide molecule detected in the interstellar medium (ISM), making it an important benchmark system for studying metal-bearing molecules in space. MgS has been observed toward the molecular cloud G + 0.693 − 0.027 near the galactic centre[5].
- Ionisation potential, bond length, polarisability, and dipole moment are calculated using optimised structure though Avogadro[2] and ORCA[4], and are presented in Table 1 along with available comparisons.
- Investigating electron interactions with MgS is essential for understanding its excitation, ionisation, and interaction mechanisms in the ISM. Accurate e^-–MgS cross-section data are therefore vital for modelling the chemistry and radiative behaviour of metal-bearing molecules in the galactic centre environment.

Methodology

- R-matrix method is an ab initio approach used for low-energy electron–molecule collisions, accurately describing elastic scattering, electronic excitation, and resonance features by dividing space into inner and outer regions[3]. We used static exchange (SE), static exchange polarisation (SEP), and the configurational interaction (CI) model in this study.
- The spherical complex optical potential (SCOP)[6] method uses a complex potential to represent scattering:

$$V_{\text{opt}} = V_{\text{st}} + V_{\text{pol}} + V_{\text{ex}} + iV_{\text{abs}}$$

  Using this optical potential, the phase shifts are obtained by solving the Schrödinger equation. The elastic and inelastic cross sections are then calculated from these phase shifts.
- The complex scattering potential-ionisation contribution (CSP-ic)[6] method estimates ionisation cross sections using an energy-dependent ratio:

$$Q_{\text{ion}} = Q_{\text{inel}} \cdot R(E)$$

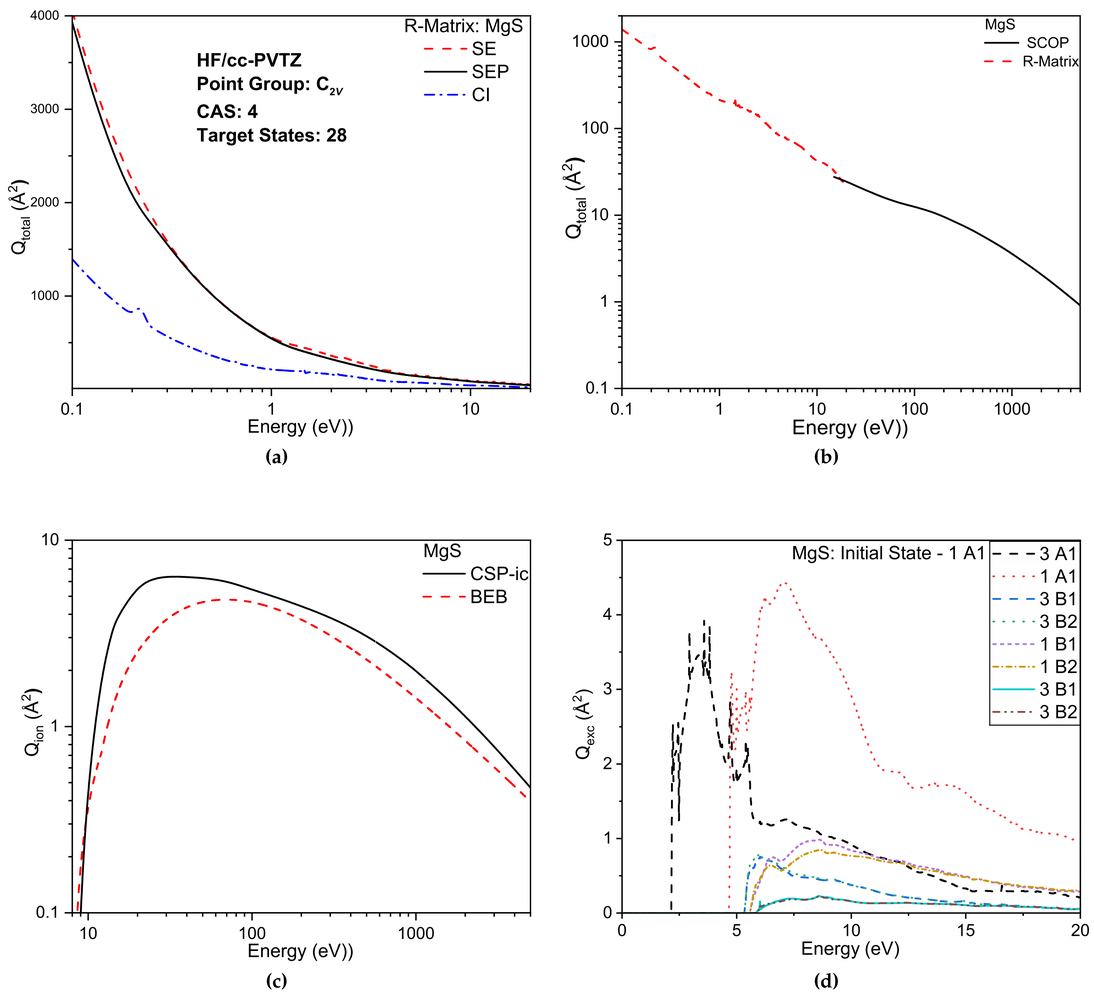
  where $R(E)$ is the scaling function, dependent on incident electron energy.
- Target properties used are calculated using the B3LYP functional and cc-pVTZ basis set, also available data from CCCBDB[1] and M. Rey *et al.*[5] given below.

Table 1: Target Properties of MgS

	IP (eV)	Bond length(Å)	α (Å^3)	μ (Debye)
Present	7.64	2.15	10.49	7.29
CCCBDB (Expt.)	–	2.14	–	–
Ref[5]	–	2.6	–	7.07

Results & Discussion

- Figure 1a shows Q_{total} from SE, SEP, and CI models. In the CI model, a hump is observed between 0.2 and 0.3 eV in the cross sections, which needs further investigation. Figure 1b shows the cross section obtained using the SCOP method, which agrees well with the R-matrix CI results around 20 eV, demonstrating the consistency of the calculations over the entire energy range.



- Figure 1c presents the Q_{ion} calculations using the BEB and CSP-ic methods. Both approaches exhibit a similar energy dependence; however, the peak of the CSP-ic cross section is shifted toward the lower energy region compared to the BEB result.
- Q_{exc} presented in figure 1d dominant contribution arises from the $^1A_1 \rightarrow {}^1A_1$ transition peak at 7 eV, which is a dipole-allowed transition, and the second dominant triplet excitation channels $^1A_1 \rightarrow {}^3A_1$ which shows strong exchange interaction at low energy. All other channels show a smaller peak and decrease slowly with energy.

Conclusion

In this study, we performed a systematic investigation of MgS and calculated elastic, inelastic, total, ionisation, and excitation cross-sections for the astrophysical molecule. We have also reported theoretical molecular properties of MgS. As the first systematic study of e^-–MgS collisions, the present results provide benchmark data for modelling and motivate further experimental and theoretical investigations.

References

[1] Cccbdb, computational chemistry comparison and benchmark database. [Online; accessed 20-January-2026].

[2] M. D. Hanwell et al. Avogadro: an advanced semantic chemical editor, visualization, and analysis platform. *J. Cheminform*, 4:22889332, 2012.

[3] T. Himani et al. Low-energy electron scattering from pyrrole and its isomers. *The Journal of Physical Chemistry A*, 127(49):10464–10480, 2023.

[4] F. Neese et al. The orca quantum chemistry program package. *J. Chem. Phys.*, 152:224108, 2020.

[5] M. Rey et al. Discovery of mgs and nas in the interstellar medium and tentative detection of cao. *The Astrophysical Journal*, 975:174, 2024.

[6] A. Yadav and B. Antony. Investigation of electron collisions with organic phosphates. *The Journal of Physical Chemistry A*, 129(34):8013–8023, 2025.